Ab initio calculation of electric-field gradients:
past, present and future

Stefaan Cottenier
Center for Molecular Modeling & Department of Materials Science and Engineering, Ghent University, Technologiepark 903, BE-9052 Zwijnaarde, Belgium

Calculating electric-field gradients from first principles has established a firm place in the research field of hyperfine interactions. In this talk, I will analyze how this has changed the way in which scientists use quadrupole interaction information. And I will argue that this is only the beginning: with fast and easy access to calculated field gradients, other ways of performing quadrupole interaction experiments will become possible.